

# Algorithm for obtaining the gradient expansion of the local density of states and the free energy of a superconductor

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(February 2, 1999)

## Abstract

We present an efficient algorithm for obtaining the gauge-invariant gradient expansion of the local density of states and the free energy of a clean superconductor. Our method is based on a new mapping of the semiclassical linearized Gorkov equations onto a pseudo-Schrödinger equation for a three-component wave-function  $\vec{\psi}(x)$ , where one component is directly related to the local density of states. Because  $\vec{\psi}(x)$  satisfies a *linear* equation of motion, successive terms in the gradient expansion can be obtained by simple linear iteration. Our method works equally well for real and complex order parameter, and in the presence of arbitrary external fields. We confirm a recent calculation of the fourth order correction to the free energy by Kosztin, Kos, Stone and Leggett [Phys. Rev. B **58**, 9365 (1998)], who obtained a discrepancy with an earlier result by Tewordt [Z. Phys. **180**, 385 (1964)]. We also give the fourth order correction to the local density of states, which has not been published before.

PACS numbers: 74.20.-z, 74.25.Bt

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## I. INTRODUCTION

The phenomenological Ginzburg-Landau theory has proven to be a powerful method to study the physical properties of superconductors in spatially varying external fields [1]. The form of the free energy  $F\{\Delta(\mathbf{r})\}$  as a functional of the complex superconducting order parameter  $\Delta(\mathbf{r})$  follows from general symmetry arguments. Alternatively, for temperatures in the vicinity of the critical temperature and for slowly varying external fields,  $F\{\Delta(\mathbf{r})\}$  can be derived microscopically from the Gorkov equations of superconductivity [2]. The microscopic approach can also be used to obtain corrections to the Ginzburg-Landau free energy functional. Tewordt [3] explicitly calculated  $F\{\Delta(\mathbf{r})\}$  up to fourth order in the gradients of  $\Delta(\mathbf{r})$ . By comparing the terms with four and two gradients, he could estimate the range of validity of the usual approximation for the Ginzburg-Landau free energy functional, where only terms with two gradients are retained. Unfortunately, a direct expansion of the free energy of a superconductor in powers of gradients of  $\Delta(\mathbf{r})$  is quite laborious, so that the result of Tewordt is rather difficult to verify, and the calculation of even higher orders seems almost impossible.

Recently Kosztin, Kos, Stone and Leggett [4], and Kos and Stone [5] (KKSL) developed new and more efficient algorithms to obtain the gradient expansion of the free energy  $F\{\Delta(\mathbf{r})\}$ . Starting point of their calculations are the Bogoliubov - de Gennes equations [6] for the two-component wave-functions and eigen-energies of a superconductor in an external field. Assuming that  $|\Delta(\mathbf{r})|$  is small compared with the Fermi energy, the low-energy physics can be obtained by linearizing the energy dispersion in the Bogoliubov - de Gennes equations. Then one arrives at the so-called semi-classical Andreev equations [7], which involve only first order derivatives. In the work [4] KKSL then use the special properties of the Andreev equations to show that for *real*  $\Delta(\mathbf{r})$  the gradient expansion of  $F\{\Delta(\mathbf{r})\}$  can be indirectly obtained from the gradient expansion of the resolvent of a one-dimensional Schrödinger operator, which is nothing but the square of the Andreev-Hamiltonian. This resolvent satisfies a non-linear second order differential equation, the so-called Gelfand-Dikii equation [4,5,8]. KKSL proceed by solving the Gelfand-Dikii equation iteratively, and then use the approximate solution to reconstruct the gradient expansion of  $F\{\Delta(\mathbf{r})\}$ . Although this strategy is more efficient than the direct approach used by Tewordt [3], this procedure still has the disadvantage that, in order to obtain all contributions to  $F\{\Delta(\mathbf{r})\}$  with  $n$  gradients, one has to calculate terms of higher order than  $n$  in the iterative solution of the Gelfand-Dikii equation. In the case of *complex*  $\Delta(\mathbf{r})$  KKSL derive a  $2 \times 2$  matrix generalization of the Gelfand-Dikii equation, which is a form of the semiclassical Eilenberger equation [9]. In this case no reshuffling of terms in the iterative procedure is necessary. To take care of a zero-mode KKSL only have to consider the next order in the gradient expansion. While in the work [4] gradients of the magnitude and the phase of  $\Delta(\mathbf{r})$  are handled separately, an expansion in terms of gradients of  $\Delta(\mathbf{r})$  itself is given in [5].

In this work we shall develop an alternative algorithm for calculating the gradient expansion of the free energy of a superconductor. We derive a pseudo-Schrödinger equation which is equivalent to the Eilenberger equation and develop a gradient expansion of the local density of states. In this expansion there appears a zero-mode which needs to be taken care of. In contrast to KKSL we fix this problem by making use of a non-linear constraint which naturally appears in our formalism. We do believe that this is an interesting and efficient

alternative to the methods developed by KKSL. Our method works equally well for real and complex  $\Delta(\mathbf{r})$  and directly generates the gradient expansion of the local density of states of the superconductor, from which the free energy can be obtained by simple integration. As an application of our method, we have explicitly calculated the local density of states  $\rho(\mathbf{r}, \omega)$  and the free energy  $F\{\Delta(\mathbf{r})\}$  up to fourth order in the gradients. We confirm the result by KKSL [4,5] for the fourth order correction to  $F\{\Delta(\mathbf{r})\}$ , who obtained a discrepancy with the expression published by Tewordt [3].

## II. FROM THE GORKOV EQUATIONS TO A PSEUDO-SCHRÖDINGER EQUATION

In this section we shall map the problem of calculating the local density of states (DOS) of a superconductor onto the problem of calculating the *time-evolution of the wave-function of an effective  $J = 1$  quantum spin in a time-dependent complex magnetic field*. For real  $\Delta$  we have recently used a similar mapping to study the effect of order parameter fluctuations in disordered Peierls chains [10]. Here we generalize this mapping to the case of complex  $\Delta$ .

### A. Reduction to an effective one-dimensional problem

Starting point of our manipulations are the Gorkov equations for the matrix Green's function of a clean superconductor in the magnetic field  $\mathbf{H}(\mathbf{r}) = \nabla_{\mathbf{r}} \times \mathbf{A}(\mathbf{r})$ ,

$$\begin{pmatrix} \omega - \mathcal{H}_{\mathbf{r}} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & \omega - \mathcal{H}_{\mathbf{r}}^* \end{pmatrix} \mathcal{G}(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}') \sigma_0, \quad (1)$$

where  $\sigma_0$  is the  $2 \times 2$  unit matrix, and the differential operator  $\mathcal{H}_{\mathbf{r}}$  is given by

$$\mathcal{H}_{\mathbf{r}} = \frac{[-i\nabla_{\mathbf{r}} + \frac{e}{c}\mathbf{A}(\mathbf{r})]^2}{2m} - \mu. \quad (2)$$

We have set  $\hbar = 1$  and measure energies and frequencies with respect to the chemical potential  $\mu$ . Here  $c$  is the speed of light and  $-e$  is the charge of an electron. Note that KKSL [4,5] start from the Bogoliubov - de Gennes equations (which are eigenvalue equations for the *wave-functions* of the superconductor) while our starting point are the Gorkov equations (which are differential equations for the *Green's functions*).

If  $|\Delta(\mathbf{r})| \ll \mu$  and if we are only interested in low-energy, long wavelength properties of the superconductor, we may linearize the energy dispersion. For calculating the local DOS and the free energy, we only need to know the Green's function at coinciding points  $\mathbf{r} = \mathbf{r}'$ . Following Waxman [11], we write

$$\mathcal{G}(\mathbf{r}, \mathbf{r}, \omega) \approx \frac{\nu_3}{\nu_1} \langle \mathcal{G}_{\mathbf{n}}(\mathbf{r}, \mathbf{r}, \omega) \rangle_{\mathbf{n}}. \quad (3)$$

Here  $\nu_d$  is the  $d$ -dimensional DOS of free fermions at the Fermi energy (including both spin directions), and  $\langle \dots \rangle_{\mathbf{n}} \equiv \int \dots \frac{d\Omega_{\mathbf{n}}}{4\pi}$  denotes directional averaging over the directions of the three-dimensional unit vector  $\mathbf{n}$ . The auxiliary Green's function  $\mathcal{G}_{\mathbf{n}}(\mathbf{r}, \mathbf{r}', \omega)$  satisfies

$$\begin{pmatrix} \omega - V(\mathbf{r}) + iv_F \mathbf{n} \cdot \nabla_{\mathbf{r}} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & \omega - V(\mathbf{r}) - iv_F \mathbf{n} \cdot \nabla_{\mathbf{r}} \end{pmatrix} \times \mathcal{G}_{\mathbf{n}}(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{n} \cdot (\mathbf{r} - \mathbf{r}')) \sigma_0 , \quad (4)$$

where  $V(\mathbf{r}) = \frac{e}{c} \mathbf{n} \cdot \mathbf{A}(\mathbf{r})$  and  $v_F$  is the Fermi velocity. Note that Eq.(4) is the Green's function analog of the Andreev equations for the wave-function [7]. Introducing  $\mathbf{r} = x\mathbf{n} + \mathbf{r}_{\perp}$  and  $\partial_x \equiv \mathbf{n} \cdot \nabla_{\mathbf{r}}$  (where  $\mathbf{n} \cdot \mathbf{r}_{\perp} = 0$ ), dropping the dependence on the parameters  $\mathbf{r}_{\perp}$  and  $\mathbf{n}$ , and setting for simplicity  $v_F = 1$ , we can write Eq.(4) as a truly one-dimensional equation,

$$\begin{pmatrix} \omega - V(x) + i\partial_x & \Delta(x) \\ \Delta^*(x) & \omega - V(x) - i\partial_x \end{pmatrix} \mathcal{G}(x, x', \omega) = \delta(x - x') \sigma_0 . \quad (5)$$

To eliminate the forward scattering potential  $V(x)$  in Eq.(5) we set

$$\mathcal{G}(x, x', \omega) = e^{-\frac{i}{2}\theta(x)\sigma_3} \mathcal{G}_1(x, x', \omega) e^{\frac{i}{2}\theta(x')\sigma_3} , \quad (6)$$

where  $\sigma_3$  is the usual Pauli matrix. Choosing the real function  $\theta(x)$  such that

$$\frac{1}{2} \partial_x \theta(x) = V(x) , \quad (7)$$

we obtain

$$\begin{pmatrix} \omega + i\partial_x & \tilde{\Delta}(x) \\ \tilde{\Delta}^*(x) & \omega - i\partial_x \end{pmatrix} \mathcal{G}_1(x, x', \omega) = \delta(x - x') \sigma_0 , \quad (8)$$

with

$$\tilde{\Delta}(x) = \Delta(x) e^{i\theta(x)} . \quad (9)$$

## B. Pseudo-Schrödinger equation for the local DOS

The gradient expansion of the free energy can be obtained from the local DOS. Because  $\mathcal{G}_1(x, x, \omega)$  has the same diagonal elements as  $\mathcal{G}(x, x, \omega)$ , the local DOS  $\rho_1(x, \omega)$  of our effective one-dimensional model can be written as

$$\rho_1(x, \omega) = -\pi^{-1} \text{ImTr}[\mathcal{G}_1(x, x, \omega + i0)] , \quad (10)$$

where due to the trace we get a factor of 2 which takes both spin directions into account. Note that in the matrix equation (8) the derivative operator  $\partial_x$  is proportional to the Pauli matrix  $\sigma_3$ . In the following it will be advantageous if the derivative operator  $\partial_x$  is proportional to the unit matrix. Using  $\sigma_3^2 = \sigma_0$ , we obtain from Eq.(8) a differential equation with this property by setting [10,5],

$$\mathcal{G}_2(x, x', \omega) = \sigma_3 \mathcal{G}_1(x, x', \omega) , \quad (11)$$

so that Eq.(8) implies

$$\begin{aligned} \left[ i\partial_x \sigma_0 + \omega \sigma_3 - \tilde{\Delta}(x) \sigma_+ + \tilde{\Delta}^*(x) \sigma_- \right] \mathcal{G}_2(x, x') \\ = \delta(x - x') \sigma_0 . \end{aligned} \quad (12)$$

For simplicity we have omitted the frequency label. The three Pauli matrices are denoted by  $\sigma_i$ ,  $i = 1, 2, 3$ , and  $\sigma_{\pm} = \frac{1}{2}[\sigma_1 \pm i\sigma_2]$ . We now generalize the method described for real  $\Delta$  in Ref. [10] to the case of complex  $\Delta$ . We start by making the *non-Abelian Schwinger-ansatz* [10,12],

$$\mathcal{G}_2(x, x') = U(x) \mathcal{G}_0(x, x') U^{-1}(x') , \quad (13)$$

where  $U(x)$  is an invertible  $2 \times 2$  matrix. It is easy to see that the solution of Eq.(12) can indeed be written in this form provided  $\mathcal{G}_0$  and  $U$  satisfy

$$[i\partial_x \sigma_0 + \omega \sigma_3] \mathcal{G}_0(x, x') = \delta(x - x') \sigma_0 , \quad (14)$$

$$\begin{aligned} i\partial_x U(x) &= \omega[U(x) \sigma_3 - \sigma_3 U(x)] \\ &+ [\tilde{\Delta}(x) \sigma_+ - \tilde{\Delta}^*(x) \sigma_-] U(x) . \end{aligned} \quad (15)$$

We parameterize  $U(x)$  as follows [10,13],

$$U(x) = e^{i\Phi_+(x)\sigma_-} e^{i\Phi_-(x)\sigma_+} e^{i\Phi_3(x)\sigma_3} . \quad (16)$$

This leads to the following system of equations for the complex functions  $\Phi_{\pm}(x)$  and  $\Phi_3(x)$ ,

$$\partial_x \Phi_+ = -2i\omega \Phi_+ + \tilde{\Delta}^* - \tilde{\Delta} \Phi_+^2 , \quad (17a)$$

$$\partial_x \Phi_- = 2i\omega \Phi_- - \tilde{\Delta}[1 - 2\Phi_+ \Phi_-] , \quad (17b)$$

$$\partial_x \Phi_3 = -i\tilde{\Delta} \Phi_+ . \quad (17c)$$

For real  $\tilde{\Delta}$  these equations reduce to the set of equations given in Ref. [10]. Recently Schopohl [13] used an analogous procedure to map the semiclassical Eilenberger equations [9] onto a similar set of non-linear equations.

The one-dimensional local DOS defined in Eq.(10) can now be written as

$$\rho_1(x, \omega) = \nu_1 \text{Re} R(x, \omega + i0) , \quad (18)$$

where the complex variable  $R(x)$  is defined by (suppressing again the frequency label)

$$R(x) = 1 - 2\Phi_+(x)\Phi_-(x) . \quad (19)$$

In principle one could now try to solve Eqs.(17a) and (17b) iteratively in powers of the derivatives of  $\tilde{\Delta}(x)$ , and then obtain the gradient expansion of the local DOS from Eqs.(18) and (19). However, the structure of the iterative solution becomes more transparent if we introduce the three-component complex vector

$$\vec{\psi}(x) = \begin{pmatrix} Z_+(x) \\ R(x) \\ Z_-(x) \end{pmatrix} = \begin{pmatrix} -\sqrt{2}[1 - \Phi_+(x)\Phi_-(x)]\Phi_+(x) \\ 1 - 2\Phi_+(x)\Phi_-(x) \\ \sqrt{2}\Phi_-(x) \end{pmatrix}, \quad (20)$$

such that the  $2 \times 2$  matrix Green's function at coinciding space points,

$$g(x) \equiv \frac{1}{2}[\mathcal{G}_2(x + 0^+, x) + \mathcal{G}_2(x, x + 0^+)] \quad (21)$$

is equal to

$$g(x) = \frac{i}{2}R(x)\sigma_3 + \frac{1}{\sqrt{2}}[Z_-(x)\sigma_+ + Z_+(x)\sigma_-]. \quad (22)$$

Because the components of  $\vec{\psi}$  can be parameterized by only two variables  $\Phi_{\pm}$ , they satisfy a constraint. Introducing the row vector

$$\tilde{\psi}^T(x) = [-Z_-(x), R(x), -Z_+(x)], \quad (23)$$

the constraint can be simply written as

$$\tilde{\psi}^T(x)\vec{\psi}(x) = R^2(x) - 2Z_+(x)Z_-(x) = 1, \quad (24)$$

which can also be expressed as

$$g^2(x) = -\frac{1}{4}\sigma_0. \quad (25)$$

Differentiating the vector  $\vec{\psi}(x)$  we find the equation of motion

$$-\partial_x \vec{\psi}(x) = H(x)\vec{\psi}(x), \quad (26)$$

with the pseudo-Hamiltonian given by

$$H(x) = \begin{pmatrix} 2i\omega & \sqrt{2}\tilde{\Delta}^*(x) & 0 \\ \sqrt{2}\tilde{\Delta}(x) & 0 & \sqrt{2}\tilde{\Delta}^*(x) \\ 0 & \sqrt{2}\tilde{\Delta}(x) & -2i\omega \end{pmatrix}. \quad (27)$$

Note that  $H(x)$  can also be written as

$$H(x) = 2i\omega J_3 + \tilde{\Delta}(x)J_- + \tilde{\Delta}^*(x)J_+, \quad (28)$$

where the  $J_i$  are spin  $J = 1$  operators in the representation

$$J_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad J_+ = \sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = J_-^\dagger. \quad (29)$$

Using the alternative parameterization of  $\vec{\psi}(x)$  in terms of the  $2 \times 2$  matrix  $g(x)$  given in (22), we find that our pseudo-Schrödinger equation is equivalent to the Eilenberger equation,

$$\partial_x g(x) = [i\omega\sigma_3 - i\tilde{\Delta}(x)\sigma_+ + i\tilde{\Delta}^*(x)\sigma_-, g(x)] . \quad (30)$$

This can be seen by using the commutation relations for the Pauli matrices and reducing Eq. (30) to the equation of motion (26). Thus we have found an unconventional derivation of the Eilenberger equations which is based on the non-Abelian Schwinger-ansatz.

Formally Eq.(26) looks like the imaginary time Schrödinger equation for a  $J = 1$  quantum spin subject to an imaginary time-dependent magnetic field. Recall that the real part of the second component of the state  $\vec{\psi}(x)$  can be identified with the local DOS. Because our pseudo-Schrödinger equation is linear, the gradient expansion of the local DOS can now be generated by a straightforward iterative calculation of the state  $\vec{\psi}(x)$  in powers of gradients. Let us emphasize that, apart from the semiclassical approximation (Eq.(3)), so far no approximation has been made. We have simply mapped the original problem onto an effective pseudo-Schrödinger equation, which is the most convenient starting point for setting up the gradient expansion.

### III. RECURSIVE ALGORITHM AND GRADIENT EXPANSION

The gradient expansion of the local DOS is directly obtained from the second component of the gradient expansion of  $\vec{\psi}(x)$ . For convenience we develop the gradient expansion of  $\vec{\psi}(x)$  for imaginary frequencies  $\omega = iE$ , because then our pseudo-Hamiltonian (27) is Hermitian and left and right eigenvectors are identical. Suppose we expand the solution of Eq.(26) in the form

$$\vec{\psi}(x) = \sum_{n=0}^{\infty} \vec{\psi}_n(x) , \quad (31)$$

where by definition  $\vec{\psi}_n(x)$  involves  $n$  derivatives with respect to  $x$ . Obviously

$$H(x)\vec{\psi}_0(x) = 0 , \quad (32)$$

i.e.  $\vec{\psi}_0(x)$  must be an eigenvector of  $H(x)$  with eigenvalue zero. The existence of such an eigenvector follows trivially from the fact that our pseudo-Hamiltonian (28) can be interpreted as the Zeeman-Hamiltonian of a  $J = 1$  quantum spin in an external magnetic field. Note that Eq.(32) determines  $\vec{\psi}_0(x)$  only up to an overall multiplicative factor, which is fixed by requiring that the components of  $\vec{\psi}_0(x)$  satisfy the constraint (24). This yields (with  $\omega = iE$ )

$$\vec{\psi}_0(x) = \frac{1}{\sqrt{E^2 + |\tilde{\Delta}(x)|^2}} \begin{pmatrix} \frac{\tilde{\Delta}^*(x)}{\sqrt{2}} \\ E \\ -\frac{\tilde{\Delta}(x)}{\sqrt{2}} \end{pmatrix} . \quad (33)$$

For the higher order terms we obtain the simple recursion relation

$$\partial_x \vec{\psi}_n(x) = -H(x)\vec{\psi}_{n+1}(x) , \quad n = 0, 1, \dots . \quad (34)$$

Because one of the eigenvalues of  $H(x)$  vanishes, the inverse of  $H(x)$  does not exist, so that we cannot simply solve Eq.(34) by multiplying both sides by  $H^{-1}(x)$ . As a consequence, Eq.(34) determines  $\vec{\psi}_{n+1}(x)$  only up to a vector proportional to  $\vec{\psi}_0(x)$ ,

$$\vec{\psi}_{n+1}(x) = -H_{\perp}^{-1}(x)\partial_x\vec{\psi}_n(x) + c_{n+1}(x)\vec{\psi}_0(x) , \quad (35)$$

where  $H_{\perp}^{-1}(x)$  is the inverse of  $H(x)$  in the subspace orthogonal to  $\vec{\psi}_0(x)$ . Using the fact that the two non-vanishing eigenvalues of  $H(x)$  are given by  $\pm 2[E^2 + |\tilde{\Delta}(x)|^2]^{1/2}$ , we find

$$H_{\perp}^{-1}(x) = \frac{H(x)}{4[E^2 + |\tilde{\Delta}(x)|^2]} , \quad (36)$$

i.e.  $H_{\perp}^{-1}(x)$  is proportional to  $H(x)$ . To fix the constant  $c_{n+1}(x)$  in Eq.(35), we require that the components of  $\sum_{i=0}^{n+1}\vec{\psi}_i(x)$  satisfy the constraint (24). This implies

$$c_{n+1}(x) = -\frac{1}{2} \sum_{i=1}^n \tilde{\psi}_i^T(x) \vec{\psi}_{n+1-i}(x) , \quad (37)$$

where the vector  $\tilde{\psi}_i(x)$  is obtained from  $\vec{\psi}_i(x)$  by exchanging the first and third components and multiplying them by  $-1$ , see Eq.(23). For odd  $n$  we can show that  $c_n(x) = 0$ . We thus obtain an explicit and very compact recursive algorithm for calculating the gradient expansion of the local DOS. To zeroth order the vector  $\vec{\psi}(x)$  is given by Eq. (33). This corresponds to the *adiabatic* approximation of elementary quantum mechanics. The step  $n \rightarrow n+1$  is summarized as follows

- $\vec{\psi}_i$  given for  $i = 0, \dots, n$
- $\vec{\psi}_{n+1} = -H_{\perp}^{-1}\partial_x\vec{\psi}_n - \frac{\vec{\psi}_0}{2} \sum_{i=1}^n \tilde{\psi}_i^T \vec{\psi}_{n+1-i} .$

(38)

It is easy to implement this iterative algorithm on a symbolic manipulation program (such as *Mathematica*). In this way the lowest few terms in the gradient expansion can be obtained in a straightforward manner.

Given the gradient expansion of the local DOS (which can be directly obtained from the second component of  $\vec{\psi}(x)$ ), we can calculate the free energy by simple integrations. Using the fact that in the normal state  $R = 1$ , the difference between the free energy densities in the superconducting and normal state of our effective one-dimensional model at inverse temperature  $\beta$  is given by  $\nu_1 f(x)$ , where

$$\begin{aligned} f(x) &= -\frac{1}{\beta} \text{Re} \left[ \int_{-\infty}^{\infty} d\omega [R(x, \omega + i0) - 1] \ln(1 + e^{-\beta\omega}) \right] \\ &= -\text{Re} \left[ \int_{-\infty}^{\infty} d\omega [N(x, \omega + i0) - \omega] \frac{1}{e^{\beta\omega} + 1} \right] \\ &= -\frac{2\pi}{\beta} \text{Im} \left[ \sum_{\omega_n > 0} N(x, i\omega_n) - i\omega_n \right] . \end{aligned} \quad (39)$$

Here  $\omega_n = (2n+1)\pi/\beta$  are fermionic Matsubara frequencies, and



$$N(x, \omega) = \int_0^\omega d\omega' R(x, \omega') . \quad (40)$$

Note that  $\nu_1 \text{Re}[N(x, \omega + i0)]$  is the integrated one-dimensional local DOS. In Eq.(39) we have used the fact that  $R(x, \omega)$  is analytic in the upper half of the complex  $\omega$ -plane. The local DOS of the three-dimensional superconductor is then given by

$$\rho(\mathbf{r}, \omega) = \nu_3 \langle \text{Re} R_{\mathbf{n}}(\mathbf{r}, \omega + i0) \rangle_{\mathbf{n}} , \quad (41)$$

where we have now written  $R_{\mathbf{n}}(\mathbf{r}, \omega)$  for  $R(x, \omega)$  to indicate the dependence on all parameters. Similarly we write  $f_{\mathbf{n}}(\mathbf{r})$  for  $f(x)$  and obtain for the difference between the free energies of the three dimensional system in the superconducting and normal state,

$$F\{\Delta(\mathbf{r})\} = \int d^3\mathbf{r} \left[ \nu_3 \langle f_{\mathbf{n}}(\mathbf{r}) \rangle_{\mathbf{n}} + \frac{|\Delta(\mathbf{r})|^2}{\lambda} + \frac{[\mathbf{H}(\mathbf{r}) - \mathbf{H}_e(\mathbf{r})]^2}{8\pi} \right] . \quad (42)$$

The second term is the field energy of the superconducting pair potential (where  $\lambda$  is the coupling constant of the Gorkov electron-electron interaction), and the last term is the magnetic field energy of the superconductor (where  $\mathbf{H}_e(\mathbf{r})$  is the externally applied magnetic field [9]).

The above equations allow for a simple recursive calculation of the gradient expansion of the free energy. To compare our results with Tewordt [3] and KKSL [4,5] we use Eq.(38) to calculate all terms in the gradient expansion up to fourth order. Systematically adding total derivatives to the expressions for the free energy (which do not change the bulk properties of the superconductor), we find the following expressions:

Zeroth order:

$$\rho^{(0)}(\mathbf{r}, \omega) = \nu_3 \Theta(\omega^2 - |\Delta|^2) \frac{|\omega|}{\sqrt{\omega^2 - |\Delta|^2}} , \quad (43)$$

$$F^{(0)}\{\Delta(\mathbf{r})\} = \int d^3\mathbf{r} \left[ -\nu_3 \frac{2\pi}{\beta} \sum_{\omega_n > 0} \left[ \sqrt{\omega_n^2 + |\Delta|^2} - \omega_n \right] + \frac{|\Delta(\mathbf{r})|^2}{\lambda} + \frac{[\mathbf{H}(\mathbf{r}) - \mathbf{H}_e(\mathbf{r})]^2}{8\pi} \right] . \quad (44)$$

Second order:

$$\rho^{(2)}(\mathbf{r}, \omega) = \nu_3 |\omega| \Theta(\omega^2 - |\Delta|^2) \left\langle -\frac{5}{32} \frac{[\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^2}{(\omega^2 - |\Delta|^2)^{\frac{7}{2}}} - \frac{1}{8} \frac{[(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\Delta|^2] - 3|\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2}{(\omega^2 - |\Delta|^2)^{\frac{5}{2}}} \right\rangle_{\mathbf{n}} , \quad (45)$$

$$F^{(2)}\{\Delta(\mathbf{r})\} = \nu_3 \int d^3\mathbf{r} \frac{2\pi}{\beta} \sum_{\omega_n > 0} \left\langle -\frac{1}{32} \frac{[\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^2}{(\omega_n^2 + |\Delta|^2)^{\frac{5}{2}}} + \frac{1}{8} \frac{|\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2}{(\omega_n^2 + |\Delta|^2)^{\frac{3}{2}}} \right\rangle_{\mathbf{n}} . \quad (46)$$

Fourth order:

$$\begin{aligned} \rho^{(4)}(\mathbf{r}, \omega) = \nu_3 |\omega| \Theta(\omega^2 - |\Delta|^2) & \left\langle \frac{1155}{2048} \frac{[\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^4}{(\omega^2 - |\Delta|^2)^{\frac{13}{2}}} + \frac{42}{512} \frac{[\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^2 (11 [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\Delta|^2] - 15 |\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2)}{(\omega^2 - |\Delta|^2)^{\frac{11}{2}}} \right. \\ & + \frac{7}{128} \frac{5 |\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^4 + 4 [\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2] [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^3 |\Delta|^2] - 10 [\mathbf{n} \cdot \nabla_{\mathbf{r}} (|\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2 [\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2])] + 3 [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\Delta|^2]^2}{(\omega^2 - |\Delta|^2)^{\frac{9}{2}}} \\ & \left. + \frac{1}{32} \frac{[(\mathbf{n} \cdot \nabla_{\mathbf{r}})^4 |\Delta|^2] - 5 [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2] + 5 |(\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}})^2 \Delta|^2}{(\omega^2 - |\Delta|^2)^{\frac{7}{2}}} \right\rangle_{\mathbf{n}}, \end{aligned} \quad (47)$$

$$\begin{aligned} F^{(4)} \{ \Delta(\mathbf{r}) \} = \nu_3 \int d^3 \mathbf{r} \frac{2\pi}{\beta} \sum_{\omega_n > 0} & \left\langle -\frac{35}{2048} \frac{[\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^4}{(\omega_n^2 + |\Delta|^2)^{\frac{11}{2}}} + \frac{70}{512} \frac{|\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2 [\mathbf{n} \cdot \nabla_{\mathbf{r}} |\Delta|^2]^2}{(\omega_n^2 + |\Delta|^2)^{\frac{9}{2}}} \right. \\ & + \frac{1}{128} \frac{5 |\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^4 - 10 |\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}} \Delta|^2 [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\Delta|^2] + [(\mathbf{n} \cdot \nabla_{\mathbf{r}})^2 |\Delta|^2]^2}{(\omega_n^2 + |\Delta|^2)^{\frac{7}{2}}} - \frac{1}{32} \frac{|(\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}})^2 \Delta|^2}{(\omega_n^2 + |\Delta|^2)^{\frac{5}{2}}} \left. \right\rangle_{\mathbf{n}}. \end{aligned} \quad (48)$$

Here  $\Theta(x)$  is the step function, and  $\mathbf{D}_{\mathbf{r}} = \nabla_{\mathbf{r}} + 2i\frac{e}{c}\mathbf{A}(\mathbf{r})$  is the covariant gradient. In deriving the above expressions we have used

$$|(\mathbf{n} \cdot \nabla_{\mathbf{r}})^l \tilde{\Delta}| = |(\mathbf{n} \cdot \mathbf{D}_{\mathbf{r}})^l \Delta|, \quad l = 0, 1, 2, \dots \quad (49)$$

Note that all terms in our expansion are gauge invariant. Since the terms involving an odd number of derivatives cancel after directional averaging we only presented the terms of even order. The directional averaging is easily done using

$$\langle (\mathbf{n} \cdot \mathbf{A})(\mathbf{n} \cdot \mathbf{B}) \rangle_{\mathbf{n}} = \frac{1}{3} \mathbf{A} \cdot \mathbf{B}, \quad (50)$$

$$\begin{aligned} \langle (\mathbf{n} \cdot \mathbf{A})(\mathbf{n} \cdot \mathbf{B})(\mathbf{n} \cdot \mathbf{C})(\mathbf{n} \cdot \mathbf{D}) \rangle_{\mathbf{n}} &= \frac{1}{15} [(\mathbf{A} \cdot \mathbf{B})(\mathbf{C} \cdot \mathbf{D}) \\ &+ (\mathbf{A} \cdot \mathbf{C})(\mathbf{B} \cdot \mathbf{D}) + (\mathbf{A} \cdot \mathbf{D})(\mathbf{B} \cdot \mathbf{C})]. \end{aligned} \quad (51)$$

Because after directional averaging the above expressions look even more complicated, we do not give the explicit results in this work. Comparing Eq.(48) with the fourth order correction to the free energy given by Tewordt [3] and by KKSL [4,5], we find that our result agrees with that of KKSL (up to a total derivative which eliminates the first term on the right-hand-side of Eq. (48)). We have not been able to find in the published literature an explicit expression for the fourth order correction to the gauge invariant local DOS, so that we cannot compare Eq.(47) with the results of other authors.

#### IV. CONCLUSION

We have developed an efficient algorithm for calculating the gradient expansion of the local DOS and the free energy of a superconductor in an external magnetic field. The linearization of the energy dispersion allows to obtain the local DOS directly from the second component of a three component wave-function  $\vec{\psi}(x)$  satisfying a pseudo-Schrödinger

equation, which is formally identical to the Schrödinger equation of a  $J = 1$  quantum spin in a time-dependent complex magnetic field. The gradient-expansion of this pseudo-Schrödinger equation turns out to be quite simple and straightforward and can be easily implemented on a symbolic manipulation program such as *Mathematica*. It seems to us that our algorithm gives an interesting alternative to the algorithms developed by KKSL [4,5]. Our final result for the contribution to the gauge-invariant free energy containing four gradients agrees with KKSL [5] and is in disagreement with the expression given by Tewordt [3]. We believe that our algorithm could also prove advantageous in other problems where fluctuation effects can be mapped onto a  $2 \times 2$  matrix equation for a Green's function in external fields. One interesting example are two coupled Tomonaga-Luttinger models.

We would like to thank Simon Kos for pointing out to us that our pseudo-Schrödinger equation is in fact equivalent to the Eilenberger equation. This work was financially supported by the DFG (Grants No. Ko 1442/3-1 and Ko 1442/4-1).

## REFERENCES

- [1] See, for example, M. Tinkham, *Introduction to Superconductivity*, (Mc Graw-Hill, New York, second edition 1996).
- [2] See, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, (Dover, New York, 1963), chapter 7.
- [3] L. Tewordt, Z. Phys. **180**, 385 (1964).
- [4] I. Kosztin, S. Kos, M. Stone, and A. J. Leggett, Phys. Rev. B **58**, 9365 (1998).
- [5] S. Kos and M. Stone, cond-mat/9809182.
- [6] P. G. de Gennes, *Superconductivity of Metals and Alloys*, (Benjamin, New York, NY, 1966).
- [7] A. F. Andreev, Zh. Eksp. Teor. Fiz. **46**, 1823 (1964) [Sov. Phys. JETP **19**, 1228 (1964)].
- [8] I. M. Gelfand and L. A. Dikii, Russian Math. Surveys **30**, 77 (1975).
- [9] G. Eilenberger, Z. Phys. **180**, 385 (1964); Z. Phys. **182**, 427 (1965); Z. Phys. **214**, 195 (1968).
- [10] L. Bartosch and P. Kopietz, Phys. Rev. Lett. **82**, 988 (1999).
- [11] D. Waxman, Ann. Phys. (N.Y.) **223**, 129 (1993).
- [12] J. Schwinger, Phys. Rev. **128**, 2425 (1962).
- [13] N. Schopohl, cond-mat/9804064.